MACHINE LEARNING BASED INTERACTION FORCE AND COLLISION MODELS FOR IRREGULAR SHAPED PARTICLES IN GAS-SOILD FLOWS

Soo hw a n Hwang, Jianhua Pan, and Liang-Shih Fan
Gas-Solid system

Liang-Shih Fan, Principles of gas-solid flows (1999)
Long He et al., Powder Technology 345 (2019)

Interaction forces

Machine Learning

DNS

Fluidized bed
Irregular shaped particles

• Require to involve complicated geometrical factors sphericity, flatness, elongation and circularity, etc.
• Most force correlations are limited to simplified or regular shaped particle
• Require heavy computation for the collision
• Neural network approach
• Interaction force: Drag, lifting, Torque
• Collision contact properties: Contact point, norm, inter-penetration depth

Vinay V. Mahajan et al., Chemical Engineering Science, 192 (2018)
Interaction Force Model
Background

- Roughness
- Elongation
- Flatness
- Orientation

Irregular shaped

A single fixed particle in low Re flow

SH : Spherical Harmonic method
VAE : Variational Auto-Encoder
PR-DNS : Particle Resolved Direct Numerical Simulation
ANN : Artificial Neural Network
Spherical Harmonic (SH) Method

- Spherical harmonic functions

\[
\begin{pmatrix}
    x(\theta, \phi) \\
    y(\theta, \phi) \\
    z(\theta, \phi)
\end{pmatrix} =
\begin{pmatrix}
    \sum_{l=1}^{l_{\text{max}}} \sum_{m=-l}^{l} C_{x,l}^m Y_l^m(\theta, \phi) \\
    \sum_{l=1}^{l_{\text{max}}} \sum_{m=-l}^{l} C_{y,l}^m Y_l^m(\theta, \phi) \\
    \sum_{l=1}^{l_{\text{max}}} \sum_{m=-l}^{l} C_{z,l}^m Y_l^m(\theta, \phi)
\end{pmatrix}
\]

- Few shape factors
  - \(d\): spherical descriptor, roughness
  - \(EI\): elongation index
  - \(FI\): flatness index
- Randomness, \(C_i = f_i(d, X \sim U(0, 1))\)

\(d = 0.5, FI = 1, EI = 1\)
Variational Auto-Encoder (VAE)

- Voxel input
- Deep CNN layers with ELUs
- Latent vectors with 128 dimension
- 2,000 datasets to train, 400 datasets to validate
- Less than 1% reconstruction error
- For the DNS, new 5,200 particles were generated (error < 1%)
PR-DNS Development

- Simplified Spheric Gas Kinetic Scheme (GKS)
- Immersed boundary Method (IBM) / Direct Forcing
- Adaptive Mesh Refinement (AMR)

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{g-f}{\tau}
\]

\[
f(0, t) \approx g(0, t) + \frac{\tau}{\delta t} (g(-\nu\delta t, t - \delta t) + g(0, t))
\]

\[
F = \int f(0, t) v_x \Xi d\mathbf{v} \quad \Xi = \begin{pmatrix} 1 \\ \mathbf{v} \end{pmatrix}
\]

\[
\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \mathbf{F} = 0, \quad \mathbf{W} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \end{pmatrix}
\]

\[
g = \begin{cases} 
\frac{\rho}{4\pi}, & \text{if } (\mathbf{u} - \mathbf{v})^2 = c^2 \\
0, & \text{otherwise}
\end{cases}
\]
DNS to ANN

- 5,200 datasets in low Re regime (0.1~10)
- Show the typical Re-$C_d$ trend, $C_d$ and $C_t$ depend on $d$, $C_l$ depends on $AR$
- 1,000~4,000 datasets for training and 1,200 datasets for validation and evaluation
ANN results

- MSEs for eq (1) is 21.8 which is comparable to the ANN result (12.7±2.7)
- MAPE of $C_d$ is 4.5% which is lower than 11.8% from eq (1)

\[
C_d = \frac{24}{ReK_1} \left\{ 1 + 0.1118(ReK_1K_2)^{0.6567} \right\} + \frac{0.4305K_2}{1 + 3305 \frac{ReK_1K_2}{ReK_1K_2}} \\
K_1 = \left[ \left( \frac{d_n}{3Deq} \right) + 2/3\psi^{-0.5} \right]^{-1}, \quad K_2 = 10^{1.8148(-log\psi)^{0.5743}}
\] (1)

G.H. Ganser, Powder Technology. 77 (1993)
ANN results

- 3 particles ($d = 0, 0.25, 0.5$)
- More accurate prediction on the lifting force and torque coefficients.

$$C_d = \frac{a_1}{Re^{a_2}} + \frac{a_3}{Re^{a_4}} + \left(\frac{a_5}{Re^{a_6}} + \frac{a_7}{Re^{a_8}} - \frac{a_1}{Re^{a_2}} - \frac{a_3}{Re^{a_4}}\right)\sin(\theta)^{a_9}$$

$$C_l = \left(\frac{b_1}{Re^{b_2}} + \frac{b_3}{Re^{b_4}}\right)\sin(\theta)^{b_5+b_6Re^{b_7}}\cos(\theta)^{b_8+b_9Re^{b_{10}}} \tag{2}$$

$$C_t = \left(\frac{c_1}{Re^{c_2}} + \frac{c_3}{Re^{c_4}}\right)\sin(\theta)^{c_5+c_6Re^{c_7}}\cos(\theta)^{c_8+c_9Re^{c_{10}}}$$

Collision Model
Collision algorithms in CFD-DEM

- DEM method involves iterative calculations for particles

1. **Mesh, IC**
2. **Compute Gas field (NS & Continuity)**
3. **Contact detect**
4. **Compute Interaction forces Ex. Drags**
5. **Calculate total forces**
6. **Update positions**
7. **Compute Collision forces**

$t_i \rightarrow t_{i+1}$
Collision algorithms in CFD-DEM

- At \( t = t_i \) and for \( j^{th} \) particle,

  1. Calculate “in or out” for \( k^{th} \) vertex
  2. \( N, k \rightarrow k+1 \)
  3. \( \text{in?} \)
  4. \( k = \text{max?} \)
  5. Calculate mean point & norm
  6. Calculate \( \delta \) with the mean norm
Non-spherical particles

• Regular & irregular particles

\[ \left( \frac{x}{r_1} \right)^2 / \varepsilon_1 + \left( \frac{y}{r_2} \right)^2 / \varepsilon_1 + \left( \frac{z}{r_3} \right)^2 / \varepsilon_1 = 1 \]

\[ x = r_1 \text{sign}(\cos \varphi_1) |\cos \varphi_1|^{\varepsilon_1} |\cos \varphi_2|^{\varepsilon_2} \]

\[ y = r_2 \text{sign}(\sin \varphi_1) |\sin \varphi_1|^{\varepsilon_1} |\cos \varphi_2|^{\varepsilon_2} \]

\[ z = r_3 \text{sign}(\sin \varphi_2) |\sin \varphi_2|^{\varepsilon_2} \]

\[ \dot{x} = \frac{2}{\varepsilon_2} \left( \left( \frac{|x|}{r_1} \right)^{\varepsilon_1} - \frac{r_1 - r_2}{r_1} \left( \frac{|x|}{r_2} \right)^{\varepsilon_2} \right) \]

\[ \dot{y} = \frac{2}{\varepsilon_2} \left( \left( \frac{|y|}{r_2} \right)^{\varepsilon_2} - \frac{r_2 - r_3}{r_2} \left( \frac{|y|}{r_3} \right)^{\varepsilon_3} \right) \]

\[ \dot{z} = \frac{2}{\varepsilon_2} \left( \frac{|z|}{r_3} \right)^{\varepsilon_3} \]

\[ \mathbf{n} = (n_x, n_y, n_z) = \frac{n}{|n|} = \frac{1}{N_1} \sum_{i=1}^{N_1} \frac{\mathbf{x}_{1,i}}{A_1} + \frac{1}{N_2} \sum_{j=1}^{N_2} \frac{\mathbf{x}_{2,j}}{A_2} \]
ANN model

• Correlate the relative position, rotational angle and vertices to contact properties.
• Two ANN models for the detection and to properties.

\[
\begin{align*}
H_p(q) &= - \frac{1}{N} \sum_{i=1}^{N} y_i \cdot \log(p(y_i)) + (1 - y_i) \cdot \log(1 - p(y_i)) \\
MSE &= \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2
\end{align*}
\]
ANN results

- 80,000 datasets
- More accurate prediction compared to volume equivalent sphere
- Rapid calculations

<table>
<thead>
<tr>
<th>Case</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact frequency ratio</td>
<td>49.40%</td>
<td>33.50%</td>
<td>33.30%</td>
<td>41.90%</td>
<td>49.50%</td>
<td>59.80%</td>
</tr>
<tr>
<td>Accuracy of the detection model</td>
<td>96.70%</td>
<td>96.20%</td>
<td>97.70%</td>
<td>96.80%</td>
<td>97.70%</td>
<td>97.50%</td>
</tr>
<tr>
<td>Accuracy assuming spheres</td>
<td>76.80%</td>
<td>76.30%</td>
<td>83.30%</td>
<td>96.60%</td>
<td>91.50%</td>
<td>89.30%</td>
</tr>
<tr>
<td>MSEs from the contact model</td>
<td>0.005</td>
<td>0.008</td>
<td>0.0067</td>
<td>0.004</td>
<td>0.0016</td>
<td>0.0045</td>
</tr>
<tr>
<td>MSEs assuming spheres</td>
<td>0.0653</td>
<td>0.0626</td>
<td>0.0802</td>
<td>0.0008</td>
<td>0.0204</td>
<td>0.0914</td>
</tr>
<tr>
<td>Sphericity</td>
<td>0.92</td>
<td>0.8</td>
<td>0.84</td>
<td><strong>0.98</strong></td>
<td>0.91</td>
<td>0.74</td>
</tr>
</tbody>
</table>
• This study provides the interaction force and collision models for the non-spherical particles.

• In DEM, the NN based models can be implemented to obtain the interaction forces and collision forces.

• Both models show high accuracy of prediction on the forces and collision properties.

• The collision model can improve the computation efficiency.
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